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Sensitivity Analysis of RELMAP (REgional Lagrangian Model of Air Pollution) Involving Fine and Coarse Particulate Matter

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16. ABSTRACT

The REgional Lagrangian Model of Air Pollution (RELMAP) is a mass-conserving, regional scale, Lagrangian model that simulates ambient concentrations as well as wet and dry deposition of SO_2, $SO_4^=$, and more recently fine (diameters< 2.5 μm) and coarse (2.5 < diameter < 10.0 μm) particulate matter over the eastern third of the United States and southeastern Canada. The simulations of fine and coarse particulate matter, which involve simple parameterizations, were recently incorporated into the model in response to impending federal regulatory standards for inhalable particulate matter and the subsequent need for size discriminate models. These new parameterizations, which include the transformation of SO_2 into $SO_4^=$, and the wet and dry deposition of fine and coarse particulate matter were allowed to vary within ± 50% of their respective nominal values in order to determine the model's sensitivity to them. Graphical analysis of the resulting ambient concentrations of fine and coarse particulate matter revealed that the model was by far most sensitive to wet deposition. Inducing a 50% variance in the wet deposition resulted in a 30 to 50% variation in the model's output concentration. A 50% variance in the dry deposition resulted in an average of 5 to 10% variation in the output, while a 50% variance in the transformation rate produced a 6 to 12% variation in the output. Future research should concentrate on refining the wet deposition parameterizations, as they not only prove to be the most influential in the model's output, but they are also currently the least understood.

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A SENSITIVITY ANALYSIS OF RELMAP INVOLVING FINE AND COARSE PARTICULATE MATTER

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1.0 INTRODUCTION

During the late 1970's, the U.S. Environmental Protection Agency (EPA) sponsored SRI International to adapt and apply their EUropean Regional Model of Air Pollution (EURMAP) to eastern North America. Like its predecessor, the new model, called the Eastern North American Model of Air Pollution (ENAMAP), simulated monthly SO_2 and $SO_4^=$ concentrations and wet and dry deposition patterns. During the early 1980's, EPA modified and improved the model in order to increase its flexibility and scientific credibility. By 1985, simple parameterizations of processes involving fine (diameters <2.5 μm) and coarse (2.5 μm < diameter < 10.0 μm) particulate matter were incorporated into the model in response to impending federal standards for inhalable particulate matter. This most recent version of the model, called the REgional Lagrangian Model of Air Pollution (RELMAP), is now capable of simulating concentration and wet and dry deposition patterns of fine and coarse particulate matter as well as SO_2 and $SO_4^=$.

These new, simplified parameterizations, which are designed to simulate the complex meteorological and chemical processes involving fine and coarse particulate matter, are only accurate to a limited degree. Because of this, they may be upgraded or even replaced in the future with more sophisticated parameterizations as further research is undertaken. As an initial step in this possible parameterization refinement, RELMAP was subjected to a "local" sensitivity analysis. In this analysis, variations found in the model's output (concentrations of fine and coarse particulate matter are considered here) due to changes in the model's parameterizations are examined, one-at-a-time, while all other input parameters are held fixed. The purpose of this paper is to present the preliminary results of this sensitivity analysis, identifying which parameterizations research should be focused upon.

2.0 MODEL BACKGROUND

RELMAP is a mass-conserving, regional-scale Lagrangian model that performs simulations upon a latitude-longitude grid which covers the eastern two-thirds of the United States and southeastern Canada as depicted in Figure 1. For an indepth discussion concerning the various attributes of the model, one is referred to the user's guide (Eder, et al., 1986).

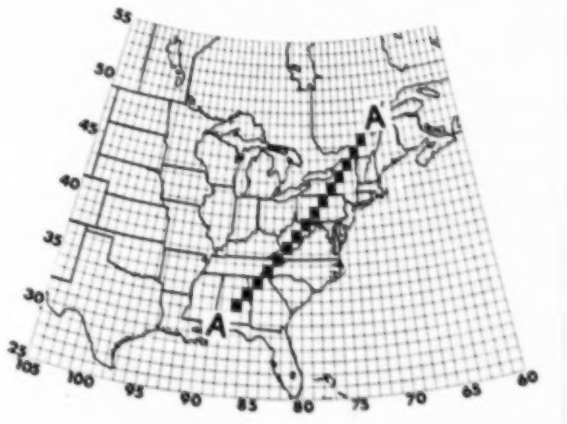

Fig. 1. RELMAP's 45°x30° domain with sensitivity analysis transect.

The model divides the atmospheric boundary layer into three layers into which seasonal emissions are injected. Discrete puffs of SO_2, $SO_4^=$ and fine (excluding $SO_4^=$) and coarse particulate matter are released every 12 hours for each of the 1350, 1° x 1° grid cells that contain sources. These puffs are subjected to linear chemical transformation and wet and dry deposition processes as they are transported across the model's domain. For each time step the suspended mass and deposition of each puff is apportioned into the appropriate grid cell based upon the percentage of puff over that grid cell. The rate of change in mass of the pollutants resulting from the transformation and deposition processes is proportional to the total mass and is defined through the following linear equations:

$$SO_2: \quad \frac{dM_1}{dt} = -M_1(Kt + Kd_1 + Kw_1) \; ; \qquad (1)$$

$$SO_4^=: \quad \frac{dM_2}{dt} = -M_2(-3/2Kt + Kd_2 + Kw_2) \; ; \qquad (2)$$

$$\text{Fine Particulate}: \quad \frac{dM_3}{dt} = -M_3(Kd_3 + Kw_3) \; ; \qquad (3)$$

Coarse Particulate : $\frac{dM_4}{dt} = -M_4(Kd_4 + Kw_4)$; (4)

where M_i is the mass of the respective pollutant (kilotons), t is the time step (hours), Kt is the transformation rate of SO_2 into $SO_4^=$, Kd is the dry deposition rate and Kw is the wet deposition rate. The 3/2 ratio used in Eq. (2) represents the ratio of molecular weights of $SO_4^=$ and SO_2.

2.1 Transformation Rate

RELMAP treats fine and coarse particulate matter as independent, non-evolving pollutants, that is physical and chemical transformation between fine and coarse particulate matter are considered to be negligible. This premise is supported by particle size distributions obtained from monitoring data (Suggs, et al., 1981), which exhibit a strong bimodal distribution with peaks in the fine and coarse ranges and a deep gap oscillating between 1 and 5 um. RELMAP does, however, consider the transformation of SO_2 into $SO_4^=$. In the atmosphere, this rate varies primarily with solar insolation (and therefore time of day, season and latitude) and moisture content. The model simulates the transformation of SO_2 to $SO_4^=$ through the use of a heterogeneous component and a homogeneous component. The hetergeneous component accounts for the more rapid transformation processes that occur under saturated conditions, while the homogeneous component simulates transformation that occurs under dry conditions. Midday, composite transformation rates used in the model typically range between 0.5%/h during the winter at high latitudes, to nearly 4%/h at low latitudes during the summer.

2.2 Dry Deposition

Dry deposition of SO_2, $SO_4^=$ and fine and coarse particulate matter is a highly variable, complex process that is parameterized by RELMAP as a function of predominant land use, stability and season. Twelve land use categories, defined by vegetation type and surface characteristics (Shein, et al., 1979) have been assigned to the model's 1° x 1° grid. Dry deposition velocities, which represent the downward surface flux divided by the local concentration, were calculated for each land use type, for six different stability classes and for each season for SO_2, $SO_4^=$ and fine and coarse particulate matter. The dry deposition velocities, which are measured in cm/s, are converted by the model into dry deposition rates (%/h). These velocities generally range between 0.05 and 1.15 cm/s for SO_2, and between 0.05 and 0.50 cm/s for both $SO_4^=$ and fine particulate matter. During the nighttime hours, the dry deposition velocities are reduced to 0.07 cm/s for SO_2, $SO_4^=$ and fine particulate matter, in order to compensate for the very high nocturnal resistance that occurs when plant absorption is minimal.

Unlike SO_2, $SO_4^=$ and fine particulate matter, the dry deposition velocities for coarse particulate matter, which range between 0.40 and 6.00 cm/s, are much less dependent upon the time of day and season. Therefore, diurnal and seasonal variations are considered negligible.

2.3 Wet Deposition

The complex process of wet deposition of SO_2, $SO_4^=$ and fine and coarse particulate matter is thought to be a function of pollutant concentration, cloud chemistry and cloud type, as well as the precipitation rate and type. RELMAP, however, parameterizes wet deposition quite simply, treating it as a function of cloud type and precipitation rate only. The wet deposition rates, which are expressed as percentages/hour, are based upon the work of Scott (1978) and consider three cloud types: Bergeron or cold-type clouds, warm or maritime-type clouds, and convective type clouds. RELMAP assumes that all winter precipitation results from Bergeron type clouds, that spring and fall precipitation results from warm cloud formation, and that summer precipitation is produced by convective type clouds. Wet deposition rates for a constant precipitation rate of 5 mm/hr can range between 2%/h during the winter to 14%/h during the summer for SO_2, and between 6%/h during the winter to 27%/h during the summer for $SO_4^=$, fine and coarse particulate matter.

3.0 SENSITIVITY ANALYSIS

The sensitivity analysis, which used real meteorological and emission data for July 1980, was performed using the currently accepted values for all input parameters. Meteorological data were obtained from the National Climatic Data Center in Asheville, NC, while the emissions data were from the 1980 National Acid Precipitation Assessment Program (NAPAP) Task Group B emission inventory (Version 4.0) and from the Environment Canada emissions inventory, used in Phase III of the U.S./Canadian Memorandum of Intent on Transboundary Air Pollution.

The parameterizations examined in the sensitivity analysis include the transformation rate of SO_2 into $SO_4^=$, and the wet and dry deposition rates of fine (including $SO_4^=$) and coarse particulate matter and SO_2 (SO_2 parameterizations are included in this analysis because SO_2 is a precursor to $SO_4^=$ and therefore fine particulate matter). With each simulation, the values of the respective parameterizations were allowed to vary ±50% around their currently accepted (nominal) values. The single value of 50% was selected for two reasons. First, choosing a single value maintains consistency and allows intercomparisons between the tests. Secondly, 50% was found to best represent the approximate lower and upper limits of the realistic changes found in all the parameters. As a result, one would expect that the subsequent changes found in the simulations of fine and coarse particulate matter concentrations would correctly represent the range in which the actual concentrations would vary, given that the exact chemistry had been incorporated into the model.

Results of the analysis were recorded for a specific transect that stretched across the model's domain (Fig. 1) from central Alabama to southern Quebec. The 15 grid cells that form this transect were chosen because they provide a good representation of the actual range of concentration values found for both fine and coarse particulate matter in eastern North America. Results from each of the seven tests are presented graphically in Figures 2 and 3. Figure 2 presents the sensitivity of

coarse particulate matter concentration to changes in the wet and dry deposition of coarse particulate matter. Figure 3 depicts the sensitivity of fine particulate matter concentration to changes in the transformation rate of SO_2 to $SO_4^=$, and to changes in the wet and dry deposition of SO_2 and fine particulate matter. Although the model treats $SO_4^=$ and fine particulate matter as mutually exclusive pollutants, the two are combined as one in this graphical analysis and simply referred to as fine particulate matter, unless otherwise noted. Each analysis consists of two graphs, with the first depicting a transect of the concentration field for either fine or coarse particulate matter. The abscissa for all plots represent the fifteen grid cells that form the transect from A to A'. The second graph depicts the percent difference with respect to the base case for each of the simulations. It should be noted that the values on each ordinate for these plots vary significantly, depending upon the parameter and the model's sensitivity to that parameter.

In each case, the asterisk represents the concentrations (fine and coarse particulate matter) that result when the parameterization being tested is reduced to 50% of its nominal value. The diamond represents the base case, where the parameter is left at its nominal value, and the circle represents 150% of the parameter's nominal value. Caution should be taken when examining the percent-difference plots over Canada (grid cells 14 and 15). Concentrations here are so small (in part due to lack of particulate matter emissions data in the Canadian inventory) that even a minute change in the magnitude of the concentration can result in greatly exaggerated percent difference values with respect to the base case.

3.1 Coarse Particulate Matter Concentrations

Examination of Figure 2 reveals that increasing either the wet or dry deposition of coarse particulate matter results in a decrease in the concentration, and that this decrease is much more sensitive to wet deposition than to dry deposition. It can also be seen that the basic spatial pattern of the concentration remains the same (i.e., the location of the local maxima and minima remain stationary), which was a common characteristic among all of the analyses. It is interesting to note, however, that the changes in the magnitude of the concentration patterns proved to be non-linear. That is, the changes in the model output were not directly proportional to changes in the input, and in most cases they proved to be far less than 50%. This can, in part, be attributed to the fact that for a given change in one parameter (with other parameters held fixed), a compensation effect will occur, induced by the other parameters, which will reduce the response of the model to the forced variation. The non-linearity is also evident in that the difference between the base case and the low deposition rates (both wet and dry) is considerably greater than that between the base case and the high deposition rates. This is due to the different "efficiencies" exhibited by each of the parameterizations. Each parameter has a maximum rate, that once exceeded, will produce no further changes in the model's simulation. This threshold value is attained more easily for the "efficient" parameterizations (all wet deposition rates, dry deposition of coarse particulate matter, and to a limited degree the transformation rate of SO_2 to $SO_4^=$), therefore increasing their values by 50% will often result in this threshold rate being exceeded, thereby limiting the impact on the concentration.

This phenomenon is well illustrated in Figure 2. Examination of the wet deposition graphs show that for a 50% decrease in wet deposition, the concentration increases an average of 30 to 50%, but for a 50% increase in wet deposition, the concentration only decreases an average of 15 to 25%. A similar trend is evident in the dry deposition graphs, but to a lesser degree. For a 50% decrease in dry deposition, the concentration increases an average of 5 to 10%, but for a 50% increase in dry deposition, the concentration only decreases between 3 and 6%.

3.2 Fine Particulate Matter Concentrations

Examination of Figure 3, which depicts the sensitivity of fine particulate matter concentration to wet and dry deposition of SO_2 and fine particulate matter, and to the transformation of SO_2 to $SO_4^=$, reveals many of the same characteristics discussed in section 3.1. The sensitivity of the concentration to wet deposition of fine particulate matter and SO_2 (which is a precursor of $SO_4^=$ and therefore fine particulate matter) each exhibit non-linear behavior. The influence of SO_2 wet deposition, however, proves to be minimal, resulting in at most a 2% difference in the output. As expected, the wet deposition of fine particulate matter has a much larger impact on the concentration. For a 50% increase in the wet deposition of fine particulate matter, the concentration decreases an average of 15 to 30%, whereas a 50% decrease in the wet deposition resulted in a 30 to 50% increase in concentration.

Examination of the dry deposition plots for both SO_2 and fine particulate matter reveals that the sensitivity of the concentration to these less "efficient" parameterizations proves to be linear. That is, the difference found between the base case and the low dry deposition rate is equivalent to the difference between the base case and the high dry deposition rates. The influence of SO_2 dry deposition on the concentrations proved to be all but non-existent, resulting in at most a 0.5% variation. However, the impact of fine particulate matter dry deposition on the concentration, though small, is more obvious, resulting in an average difference of 2 to 5%.

And finally, as seen at the bottom of Figure 3, the sensitivity of fine particulate matter concentration to changes in the transformation rate of SO_2 to $SO_4^=$, proves to be slightly nonlinear. A 50% increase in the transformation rate increases the concentration by an average of 5 to 10%, while a 50% reduction in the transformation rate results in a 6 to 12% decrease in the concentration.

4.0 CONCLUSIONS

The effect of separately introducing ±50% variations in three major parameterizations (wet deposition, dry deposition, and transformation rate) involving the simulation of fine and coarse particulate matter concentration by RELMAP has been examined. Although the results presented here are preliminary, several important conclusions can be reached:

1) Simulated concentrations of fine and coarse particulate matter are by far, most sensitive to variations in the wet deposition rates of fine and coarse particulate matter, respectively. However, concentrations of fine particulate matter proved to be quite insensitive to wet deposition of the SO_2.

2) Concentrations of coarse particulate matter were somewhat sensitive to dry deposition of coarse particulate matter. Concentrations of fine particulate matter were, however, less sensitive to dry deposition of fine particulate matter, and were in fact highly insensitive to dry deposition of SO_2.

3) Concentrations of fine particulate matter proved to be somewhat sensitive to the transformation rate of the precursor SO_2 into $SO_4^=$.

Future research should concentrate on refining the parameterizations involving the wet deposition of both fine and coarse particulate matter. Not only has wet deposition proven to be the most influential parameterization employed by RELMAP, it is also currently the least understood. Although the model proved to be somewhat less sensitive to other parameterizations, future research will also be conducted in these areas so that they too will parameterize the essential physical and chemical processes occurring in the atmosphere more accurately.

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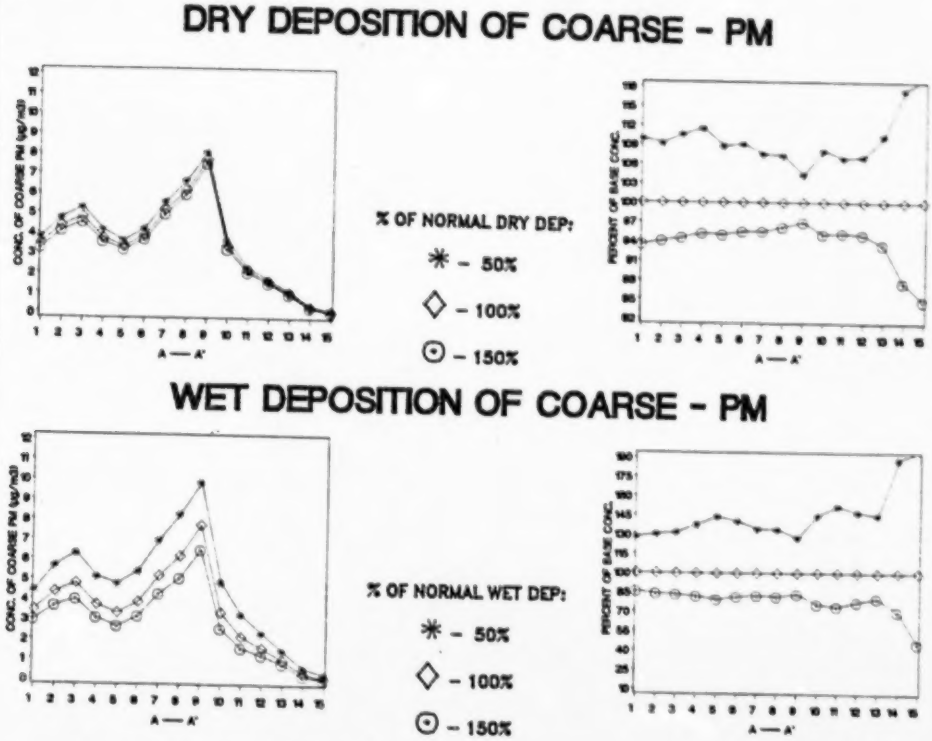

Figure 2. Sensitivity of Coarse Particulate Matter Concentrations to changes in the dry and wet deposition rates of Coarse Particulate Matter.

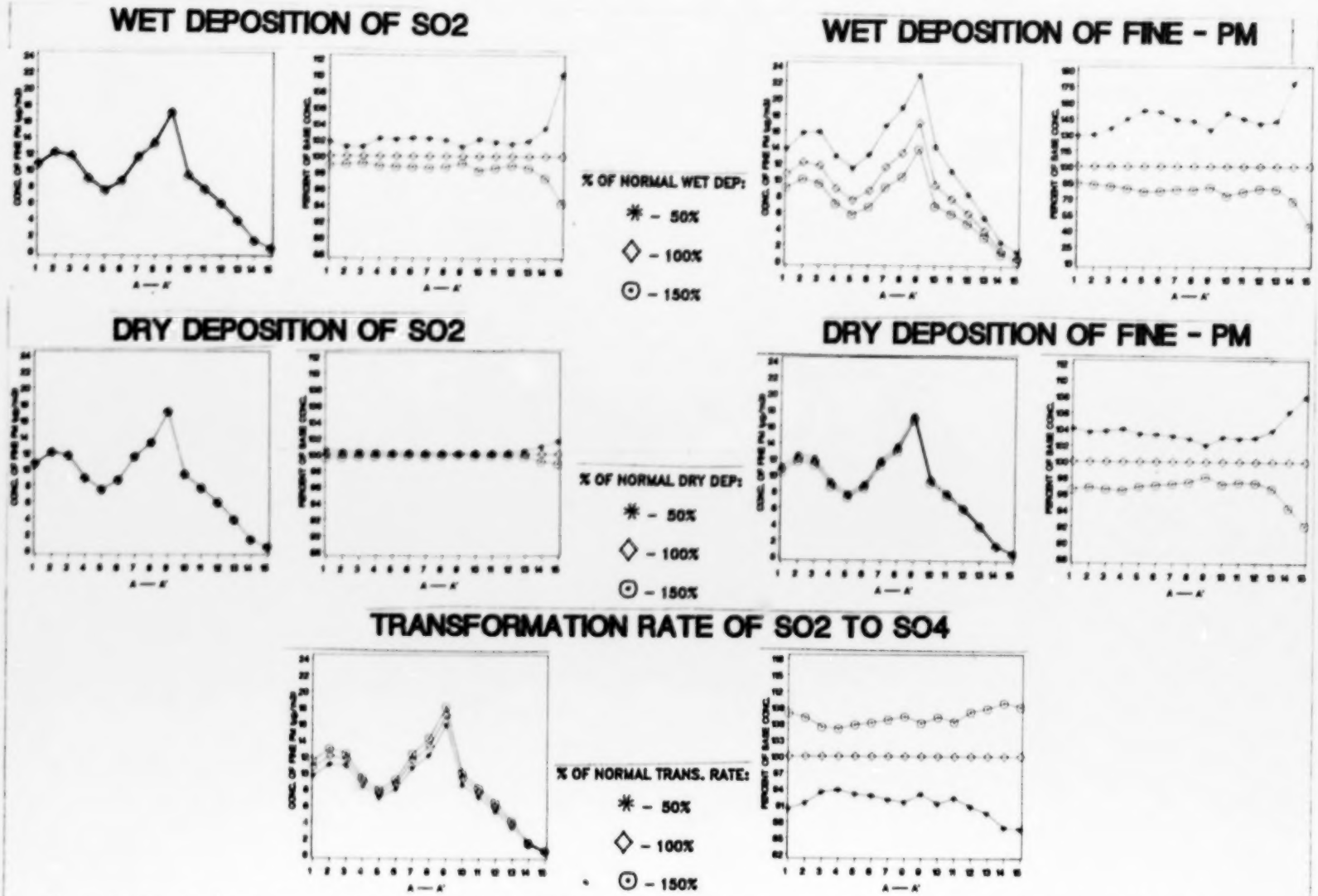
WET DEPOSITION OF SO2
WET DEPOSITION OF FINE - PM
% OF NORMAL WET DEP:
* - 50%
◇ - 100%
⊙ - 150%
DRY DEPOSITION OF SO2
DRY DEPOSITION OF FINE - PM
% OF NORMAL DRY DEP:
* - 50%
◇ - 100%
⊙ - 150%
TRANSFORMATION RATE OF SO2 TO SO4
% OF NORMAL TRANS. RATE:
* - 50%
◇ - 100%
⊙ - 150%

Figure 3. Sensitivity of Fine Particulate Matter Concentrations to changes in the wet and dry deposition of SO_2 and Fine Particulate Matter and to changes in the transformation rate of SO_2 into $SO_4^=$.